Brief Curriculum Vitae

1 Personal Details

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2 Academic Qualifications

BSc(Hons) Physics.
MSc(Lond): Nuclear Reactor Science and Engineering.
PhD(Lond) Theoretical Elementary Particle Physics.

3 Brief Summary of Career History

Present Positions
• Professor of Computational Nano-Science and Nano-Technology, and Head of Department of Medical Physics and Biomedical Engineering, Faculty of Medicine, Shahid Beheshti University of Medical Sciences.
• Professor of Computational Nano-science and Condensed Matter Physics. Founder and Head of School of Nano-Science, Institute for Research in Fundamental Sciences (IPM), Tehran/Iran.
Past Positions
• Head of Nano-Technology Committee, Ministry of Science, Research and Technology (2001-2002), Iran.

• Head of Research (1994-2000), Computational Nano-Science Research Section, Centre for Numerical Modelling and Process Analysis, University of Greenwich, England.
• Invited Research Professor in Computational Nano-Science, Institute for Materials Research (Tohoku University, Japan) 1992-1993. Now continuing on a collaborative basis.
• Research Fellow, Computational Nano-science Research Group, Department of Materials, University of Oxford, 1990-1992.
• Associate Professor in Mathematics and Computer Science, South West London College 1989-1992.
• Visiting Research Physicist in Foundation of Quantum Mechanics, Henri Poincari Institute (Paris), 1984-1987.
• United Nations (UN) Research and Educational Consultant, 1994-1995.
• Co-chair of the Physics and Economic Development Committee, World Conference on Physics and Sustainable Development, South Africa (2005) and Head of the International Network on Nanotechnology Projects, supported by UN .

4 Additional information

• PhD and MSc thesis supervisor in UK and Iran.
• Founder and Head of the Computational Nano-Science Research Group in the Centre for Numerical Modelling and Process Analysis at Greenwich University, England. Several personal research grants, including:
(a) Recipient of substantial Engineering and Physical Sciences Research Council (EPSRC)post-doctoral grant for the project to develop a multi-scale (atomistic+ continuum) modelling of fracture and crack propagation processes in crystalline and polymeric materials.
(b) Recipient of the grant under the Joint British-Polish Research Collaboration Programme from the British Council for a collaborative research with the universities of Poznan and Worclaw for a multi-scale modelling and first-principle computation, and experimental study, of the nucleation and growth of metallic and semi-conducting thin films on supporting substrates.
(c) Recipient of British Royal Society Visiting Research Fellowship grant to investigate the meso-scale modelling of stochastic processes in fluid bio-membranes.
• Invited speaker to more than 150 conferences and meetings both in the UK and 15 other countries, promoting nano-science research fields. Regular invitation to seminars at other universities. Chair of several symposia in condensed matter physics, eg. the nano-science symposium at the Liverpool Meeting of the IOP (1995).
• Acting referee for several IOP (England), Elsevier, and ACS research journals.
• External PhD examiner, PhD and post-doctoral research fellow supervisor.
• Strong collaborative links with the UK-based institutions (Birmingham and Sussex universities) and with the universities of Poznan and Worclaw (Poland) and Tohoku (Japan).
• More than 100 radio and TV interviews on various aspects of nano-scale physics and nanotechnology.
• 30 PhD and MSc-level thesis supervision in nano-science in Iran since 2002.

5 Honours and awards

• Elected Chehreyeh Mandegar (Distinguished Permanent National Science Personality) (Nano-Technology) 2006.
• Elected number one researcher in nano-technology at the first national meeting to elect the top nano-technology researchers in Iran, organised by the Iranian National Nano-Technology Committee, affiliated to the Science and Technology Directorate of the President's Office.
• Joint winner of the Elegant Work Prize of the Institute of Materials London(1994) for outstanding contribution to the investigation of nano-scale systems and processes.

6 Major research fields undertaken

My research activities can be divided into two broad fields:
(a): Foundations of Quantum Theory
(b): Computational Nano-Science and Condensed Matter Physics at the Nano-scale

(a) Foundations of Quantum Theory
This research field involves some of the fundamental issues at the foundation of theoretical quantum physics, including its application to biological systems, such as the Hameroff-Penrose model of quantum cognition processes. The aim here has been to construct a comprehensive and self-consistent model in which *classical* physical concepts, such as space-time trajectories, equations of motion etc, can be introduced into the framework of standard quantum mechanics. The standard (Copenhagen) formulation of quantum theory allows only for the computation of *probabilities* of quantum processes, and is incapable of offering any algorithm for computing, or even posing, the space-time description of quantum events, i.e. it cannot provide a *quantum theory of motion*. My research in this field, along with those of others, has led to a completely different alternative model of the quantum phenomena. This stochastic model forms a part of the *causal-stochastic model of quantum theory*, originally developed by de Broglie, Bohm and Vigier. I am still active in this field, and from time to time publish papers on various aspects of this subject. The specific topics in this field with which I have been involved with are:

◇ *The path-integral formulation of the space-time motion of quantum particles in the causal-stochastic model of quantum theory.*
◇ *Introduction of temperature into the motion of quantum particles.*

These topics, continuing on a collaborative basis and now moving into problems related to a causal-stochastic modelling of *many-body* quantum systems, were originally formulated and initiated in association with the late Professor J.P Vigier's Theoretical Physics Laboratory at the Institute Henri Poincare (Paris). Their results have led to a significant generalisation of the de Broglie-Bohm-Vigier theory of quantum phenomena.

(b): Computational Nano-Science, Nano-technology, and Condensed Matter Physics at the Nano-scale
These fields are currently at the forefront of research in nano-science, nano-technology and the related area of materials design from first principles, actively pursued in Europe, the US and Japan. It has formed the main field of my research activity over the past 20 years in both Europe, Japan and now in Iran. Within these general areas, I have been specifically involved in the following comprehensive researcg programmes

• *Modelling the tribological, adhesion, fracture, friction and indentation properties of metallic and semi-conducting nano-crystals using computer-based atomistic-level simulations*
The Modelling studies have employed a variety of simulation techniques, including Molecular Dynamics (MD), Stochastic Molecular Dynamics (SMD), and Multi-scale Modelling, using many-body inter-atomic potentials to model the energetics and dynamics of individual atoms. This was the first project in nano-science started in England (1990) in which the irreversible processes unfolding in nano-scale crystals that are subject to externally applied stresses were modelled. The project was initiated while I was at the Department of Materials (University of Oxford), and was funded by the British Research Council (EPSRC) via three substantial grants, including a grant for the purchase of a mini supercomputer on which the large-scale codes were implemented and the results were visualised. The project was the first of its type in Europe and its results led to gaining significant insights into the *nanoscopic* irreversible processes that underlie such *macroscopic* phenomena as friction, fracture and indentation of metallic systems, and the influence of adsorbate protective monolayers on their adhesive characteristics. This research was awarded the Institute of Materials (London) Elegant work Prize for 1994.

• *Development of new inter-atomic potentials*
This work, also initiated at Oxford University and was concerned with the formulation of new *many-body* interatomic potentials for the description of the energetics of the FCC random binary alloys. The research led to the construction of a novel *unified* set of potentials that model the alloy states of all the 10 FCC metals as a combination of their pure elemental states. The potentials are now referred to in the literature as the Rafii-Tabar and Sutton many-body alloy potentials.

• *Modelling the nucleation and growth of nano-phase films on supporting substrates*
This project was initiated at the Institute for Materials Research (University of Tohoku, Japan) and supported by Hitachi Corp via a Visiting Research Professorship. It continues as a collaborative effort. The Modelling employed both the *ab initio* density functional techniques and the standard MD simulation method. It is concerned with the modelling of the epitaxial growth of molecular and atomic thin films, such as C_{60} molecules and other clusters and metallic atoms, on supporting semi-conducting (eg Si), metallic and semi- metallic (such as HOPG) substrates. These substrates are of exceptional importance in the fabrication of the next generation of nano-sized devices, with wide applications in the electronic and information-technology industries. This project led to deep understanding of the physics of the molecular thin films grown on semi-conducting substrates

• *Swelling of crystals subject to thermonuclear radiation*
The project was supported by the National Centre for Fusion Studies in Japan. The atomic-scale modelling was concerned with elucidating the possible mechanisms underlying the phenomenon of *void generation* in crystals of nuclear materials, such as Vanadium, subject to intense radiation in a fusion reactor. A novel model, based on the migration of di-vacancies, was developed. The MD-level simulations led to a significant understanding of the role of crystal defects (dislocation bias) in the diffusion and growth of voids in the BCC materials under intense radiation.

• *Multi-scale modelling of crack propagation in crystalline materials*
This project, funded by EPSRC through, was concerned with the development of a completely novel model of crack propagation in materials. It involved the formulation of a *multi-scale* (atomistic+continuum) seamless stochastic model in which the nano-mechanics of the rupture of the atomic bonds at the crack tip was coupled, across several length and energy scales, with the continuum mechanics of the macroscopic stress fields applied remotely to the edges of a metallic sample of a macroscopic size. Both pure elemental metals and their random binary alloys were considered. Crack propagation over macroscopic distances in *real space* was thus modelled in terms of the data on the crack tip atom obtained at the nano-scales. The model correctly predicted the crack velocity. It generated the macroscopic random *crack trajectories*, via Ito stochastic calculus, in terms of the diffusion constant of the crack tip atom, and successfully explained the origin of the crack bifurcation and branching. The research has been recognised as making a fundamental contribution to the field of fracture modelling in solid materials. A post-doctoral research fellow was employed for this project.

• *Multi-scale modelling and experimental investigation of adsorption of atomic clusters on metallic substrate*
This is an ongoing joint project with the departments of physics at the Poznan Technical University(Poland) and Worclaw University (Poland). It was funded by a grant from the British Council under the British- Polish research collaboration. This is an extensive research programme consisting of both theoretical and experimental aspects. The theoretical part concerns the modelling of the complex process of *soft landing* and adsorption of metallic atomic clusters on substrates from a vapour phase, followed by their surface diffusion and coalescence at *elevated* time scales. It also involves first-principle calculations of the band structure of the adsorbed clusters via a Green function method based on the relativistic quantum field theory. The experimental aspect is implemented in Poland using an STM facility at Poznan.

• *Modelling the meso-scale diffusion processes in stochastic fluid bio-membranes*
This is an ongoing project in collaboration with Dr. HR Sepangi at the Physics Department of Shahid Beheshti University (Iran). It was initially funded by a British Royal Society Fellowship grant. The project, which is at the interface of theoretical physics and biology, is concerned with the development of the space-time dynamics of rigid external objects moving in a stochastically fluctuating fluid bio-membrane decorated with internal inclusions. These internal inclusions can be the protein channels to the interior of the cells. The energetics of the

membrane is described in terms of purely geometrical concepts by treating the membrane as a two-dimensional sheet over the mesoscopic scales and subsuming its molecular architecture into the background. The model, when combined with an atomistic modelling of the molecular docking of the external objects with the internal inclusions, can lead to the formulation of an algorithm suitable for designing functional membranes for targeted drug delivery, where the external objects can mimic the drug particles.

• *A comprehensive research programme on the modelling of the properties of carbon nanotubes as the most important form carbon nano-structure for nano-technology.*
The project was initiated in Iran for the first time, and has led to a large number of publications, including the book " *Computational Physics of Carbon Nanotubes*" published by the *Cambridge University Press* in 2008.

• An extensive research programme in Iran, leading to several PhD Thesis, on the application of computational modelling to the physics of nanoscopic structures in biological systems, including the investigation of electromagnetic radiation with sub-cellular structures.

• A comprehensive research programme in Iran in nano-fluidics, leading to PhD Thesis, investigating the structural stability of nano-channels during fluid transport.

• Investigation of the effects of radiation on neuronal systems, with particular emphasis on the interaction of RF radiation on the neurotransmitters and CSF.

7 Select publications relevant to nano-science and nano-technology

Books

H. Rafii-Tabar, Computational Physics of Carbon Nanotubes
Cambridge University Press, Cambridge, 2008

Chapters in Books

(1): A.P. Sutton, J.B. Pethica, H. Rafii-Tabar and J.A. Nieminen, "Mechanical properties of metals at the nanometre scale, in *Electron theory in alloy design"*(D.G. Pettifor and Sir A.H. Cottrell eds) Institute of Materials(London) (1992) 191-233. Winner of 1994 Institute of Materials Elegant Work Prize.

(2) H. Rafii-Tabar, "Nanoscopic modelling of the adhesion, indentation and fracture characteristics of metallic systems via molecular dynamics simulation, in *Mesoscopic Dynamics of Fractures: Advances in Materials Research,* eds Kitagawa, Aihara and Kawazoe (Springer Verlag, Berlin, 1998) 36-48.

(3) H. Rafii-Tabar and G.A. Mansoori, " Inter-atomic Potential Models for Nano-Structures"', *Encyclopedia of Nanoscience and Nanotechnology*, Vol IV, Edited by H.S. Nalwa, American Science Publishers, 2003.

(4) H.Rafii-Tabar, " Computational Modeling of Tribological, Adhesion, Indentation and Fracture Processes in Nano-scale Systems" *Volume 4, Handbook of Theoretical and Computational Nanotechnology (Edited by M. Rieth, and W. Schommers)*, American Scientific Publishers, 2006

(5) H. Rafii-Tabar, "Thermo-Mechanical and Transport Properties of Carbon Nanotubes"*Encyclopedia of Complexity and Systems Science, (Edited by Meyers)*, Springer Verlag, Berlin, 2008

Review Papers
(1) H. Rafii-Tabar, "Modelling the nano-scale phenomena in condensed matter physics via computer- based numerical simulations. *Physics Reports* Vol 325 (2000)239-310

(2) H. Rafii-Tabar, A. Chirazi, " Multi-scale Computational Modelling of Solidification Phenomena"',*Physics Reports* Vol 365 (2002) 145-249.

(3) H. Rafii-Tabar, "'Computational Modelling of the Thermo-Mechanical and Transport Properties of Carbon Nanotubes"'. *Physics Reports* Vol 390 (2004) 235-452.

Papers

(1) H. Rafii-Tabar, "Real Feynman-Like Stochastic Paths in Bohm-Vigier Causal-Stochastic Model of Quantum Mechanics", *Phys Lett. 138 (1989) 353-358.*

(2) H. Rafii-Tabar and A.P. Sutton, "Long-range Finnis-Sinclair potentials for fcc metallic alloys", *Phil.Mag. Lett. 63 (1991) 217-224.*

(3)H. Rafii-Tabar, J.B. Pethica and A.P. Sutton, "Influence of adsorbate monolayer on the nano-mechanics of tip-substrate interactions", *Mat. Res. Soc. Symp. Proc. vol 239 (Nix et al eds) Massachusetts (1992) 313-318.*

(4)H. Rafii-Tabar and Y. Kawazoe, "Influence of cluster size on the nano-mechanics of tip-substrate interactions", *Proc. 2nd Int. Conf. and Exn. on Computer Applications to Materials and Molecular Science and Engineering (CAMSE) (M. Doyama et al eds) Yokohama City(Japan) (1992) 627-630.*

(5) H. Rafii-Tabar and Y. Kawazoe, "Dynamics of atomically thin layers-surface interactions in tip-substrate geometry", *Japan J. Appl. Phys. vol 32 (1993)1394-1400.*

(6) Y. Kawazoe, Y. Maruyama, H. Rafii-Tabar, M. Ikeda, H. Kamiyama and K. Ohno, "Structure of layered C_{60} on Si(100) surface studied by ab initio and classical molecular dynamics simulation", *Mat. Sci. Eng. B19 (1993) 165-171.*

(7) H. Rafii-Tabar, Y. Kawazoe and H. Kamiyama, "Stability of the Fullerenes thin film deposited on the Si(100) surface", *Mat. Res.Soc. Proc. vol 308 (P.H. Townsend et al eds) San Francisco (1993) 467-471.*

(8) H. Rafii-Tabar, H. Kamiyama and Y. Kawazoe, "Dynamics of C60 Buckyballs on Si(100) surface", *Proc. Int.Conf. on computer-assisted materials design and process simulation(COMMP) Tokyo (1993) 2225.*

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(11)H. Rafii-Tabar, "Simulating the motion of a quantum particle at constant tem-

perature", *Foundations of Physics, 25,(1995) 317-328.*

(12) H. Rafii-Tabar, A.L. TambyRajah, H. Kamiyama and Y. Kawazoe, "Molecular dynamics simulation of Observed c(4x4) and c(4x3) C_{60} Alignments on Si(100) reconstructed surface", *Modelling Simul.Mater.Sci.Eng. 4,(1996) 101-110.*

(13)L. Hua, H. Rafii-Tabar and M. Cross, "Molecular dynamics simulation of fractures using an N-body potential", *Phil. Mag. Letts, 75 (1997) 237-244.*

(14) H. Rafii-Tabar, L. Hua and M. Cross, "A multi-scale numerical modelling of crack propagation in a 2D metallic plate", *J. Computer-Aided Mat. Desgn. 4 (1997) 165-173.*

(15) H. Rafii-Tabar, H. Kamiyama and M. Cross, "Molecular dynamics simulation of adsorption of Ag particles on a graphite substrate", *Surf. Sci. 385 (1997) 187-199.*

(16) H. Rafii-Tabar, L.Hua and M. Cross,"A Multi-scale atomistic-continuum modelling of crack propagation in a two-dimensional macroscopic plate",
J. Phys.:Condens.Matter 10 (1998) 2375-2387.

(17)H. Rafii-Tabar, "Numerical modelling of adsorption of metallic particles on graphite substrate via molecular dynamics simulation", *Acta Phys. Polonica A 93 (1998) 343-354.*

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(20)R. Czajka, L. Jurczyszyn and H. Rafii-Tabar, "Surface physics at the nanoscale via scanning probe microscopy and molecular dynamics simulations", *Prog. in Surf. Sci 59 (1998) 13-23.*

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(22) H. Rafii-Tabar, "Modelling the dynamics of membrane diffusion", *(cover article), Scientific Computing World, Issue 45 February/March (1999) 18-20.*

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(24) H. Rafii-Tabar, H. R. Sepangi, "Modelling meso-scale diffusion processes in stochastic fluid bio-membranes". *Computational Materials Science,15 (1999) 483-492 .*

(25) A. Chirazi and H. Rafii-Tabar, "Coupling the nano and meso scales in modelling the formation of metallic microstructures" *Mat. Res.Soc. Proc. vol 308 (P.H. Townsend et al eds) San Francisco (1999) 467-471 .*

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(28) H. Rafii-Tabar, "The Nano-Science of the C_{60} Molecule",*Iranian Journal of Physics Research, Vol 3, No 2 (2002)*

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(33) H. Rafii-Tabar, "'Computational Condensed Matter Physics at Nano-scale. *A comprehensive research textbook being written for Springer-Verlag publishers by invitation.*

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(46) H. Rafii-Tabar and R. Tavakoli-Darestani, "Modelling the stochastic dynamics of biological nano-motors: An overview of recent Results". *Journal of Computational and Theoretical Nanoscience Vol.6 (2009) 806*

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